Supporting Information

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Analysis of Shear Band Plasticity and Evaluation of Stress Intensity Factors

Using an analysis of shear band plasticity based on a model of an elastic-perfectly plastic solid, Conner et al. (26) derived an analytical expression to evaluate the stress intensity factor in bending of an unnotched metallic glass plate. In their analysis for symmetric bending of a plate having half-thickness h, the critical Mode I stress intensity factor K_{IC} is related to the bending strain at fracture ε_f according to

$$K_{IC} = \left\{ \frac{2G}{(1-\nu)} \varepsilon_y \left[\frac{3}{2} - \frac{1}{2} \left(\frac{\varepsilon_y}{\varepsilon_f} \right) \right]^2 \right\} \sqrt{\pi c} \left[1.12 - \frac{1.39}{2} \left(\frac{c}{h} \right) + \frac{7.3}{4} \left(\frac{c}{h} \right)^2 - \frac{13}{8} \left(\frac{c}{h} \right)^3 + \frac{14}{16} \left(\frac{c}{h} \right)^4 \right], \quad \textbf{[S1]}$$

where G is shear modulus, ν the Poisson's ratio, ε_y the elastic strain at yielding, and c is the length of the stable crack formed in the shear band before unstable fracture, and can be related to ε_f according to

$$c = h \sqrt{ \left[1 - \left(\frac{\varepsilon_y}{\varepsilon_f} \right) \right]^2 - \left(\frac{h\alpha}{\varepsilon_f - \varepsilon_y} \right)^2 }, \quad \textbf{[S2]}$$

where α is a curvature parameter given by

$$\alpha = \frac{(1-\nu)}{(1-2\nu)} \frac{\Delta u^*}{\sqrt{2}h^2}, \quad \textbf{[S3]}$$

where Δu^* is the critical shear offset attained in the shear band before transitioning into an unstable crack (i.e., before fast fracture). Δu^* is considered a material constant, and for typical metallic glasses is on the order of a few micrometers. In principle, Δu^* is an accessible length scale that may be measureable by microscopy. But, for the purpose of this model, Δu^* can be regarded as a model parameter that can be adjusted such that the K_{IC} evaluated by Eq. **S1** matches the measured K_{IC}.

Kumar et al. (15) tested 0.6-mm-thick metallic glass plates of $Pt_{57.5}Ni_{5.3}Cu_{14.7}P_{22.5}$, $Pd_{43}Ni_{10}Cu_{27}P_{20}$, and $Zr_{44}Ti_{11}Cu_{10}Ni_{10}Be_{25}$ in bending after annealing the plates at various relaxation temperatures T_R around the glass transition temperature T_g, and reported the strain to fracture as a function of relative temperature T_R/T_g.

The shear modulus G and Poisson's ratio ν are known to vary strongly when the glass is relaxed at different relative temperatures T_R around T_g. The temperature dependence of the shear modulus $G(T_R)$ is given by (21)

$$G(T_R) = G_g \exp\left[n\left(1 - T_R/T_g\right) \right], \quad \textbf{[S4]}$$

where G_g is the measured value of the shear modulus for a glass relaxed at T_g [i.e., $G_g = G(T_g)$] and n is a material constant related to the fragility of the glass. The bulk modulus B on the other hand is known to vary only slightly with varying T_R, an effect also corroborated in the present work (see Table 1 in the main text), and is hence considered to be a constant having the value measured in the as-cast glass state. The temperature dependence of the Poisson's ratio under this assumption is solely due to $G(T_R)$, and is given by

$$\nu(T_R) = \frac{3B - 2G(T_R)}{2(3B + G(T_R))}. \quad \textbf{[S5]}$$

For the purpose of this analysis, the critical shear offset Δu^* is a model parameter determined by requiring Eq. **S1** to produce a K_{IC} value at T_g [i.e., $K_{IC,g} = K_{IC}(T_g)$] equal to the measured value in the as-quenched glass state of each composition. In this manner, the K_{IC} values estimated from the model at various T_R are calibrated to the reported measured K_{IC} value for each composition. The critical Mode I stress intensity factor K_{IC} has been evaluated for $Pt_{57.5}Ni_{5.3}Cu_{14.7}P_{22.5}$ (33) and $Zr_{44}Ti_{11}Cu_{10}Ni_{10}Be_{25}$ (11), but no value has been reported for $Pd_{43}Ni_{10}Cu_{27}P_{20}$. Therefore, the present analysis is implemented to evaluate K_{IC} from ε_f data only in the $Pt_{57.5}Ni_{5.3}Cu_{14.7}P_{22.5}$ and $Zr_{44}Ti_{11}Cu_{10}Ni_{10}Be_{25}$ systems. Lastly, it should be noted that the K_{IC} values estimated from the model at various T_R are not necessarily "plane-strain fracture toughness" values, as the samples used in ref. 15 likely were not thick enough to ensure crack propagation in plane strain.

In the context of this analysis, only data for strain to fracture ε_f from ref. 15 that substantially exceed the material elastic yield strain ε_y are used in Eqs. **S1** and **S2**, whereas data where ε_f is close to or equal to ε_y are neglected. This is because, as noted by Conner et al. (26), Eqs. **S1** and **S2** are valid only when the strain at the plate surface is substantially high to initiate a crack at the surface.

A plot of the strain to fracture ε_f vs. T_R/T_g reported in ref. 15 for $Pt_{57.5}Ni_{5.3}Cu_{14.7}P_{22.5}$ and $Zr_{44}Ti_{11}Cu_{10}Ni_{10}Be_{25}$ is presented in Fig. S1. All model parameters used in the present analysis to evaluate K_{IC} from the reported ε_f data using Eq. **S1** for $Pt_{57.5}Ni_{5.3}Cu_{14.7}P_{22.5}$ and $Zr_{44}Ti_{11}Cu_{10}Ni_{10}Be_{25}$ are presented in Table S1. The evaluated K_{IC} data for $Pt_{57.5}Ni_{5.3}Cu_{14.7}P_{22.5}$ and $Zr_{44}Ti_{11}Cu_{10}Ni_{10}Be_{25}$ are plotted in Fig. S2 against T_R/T_g.

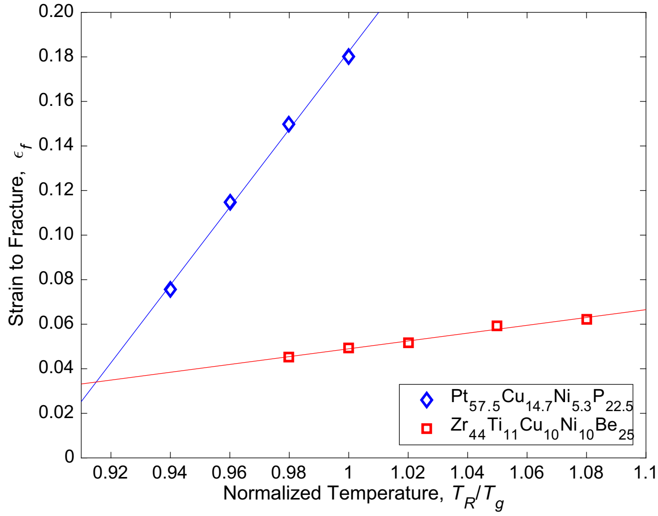

Fig. S1. Strain to fracture ε_f vs. normalized temperature T_R/T_g as reported in ref. 15 for $Pt_{57.5}Ni_{5.3}Cu_{14.7}P_{22.5}$ and $Zr_{44}Ti_{11}Cu_{10}Ni_{10}Be_{25}$. Solid lines are linear fits to the data.

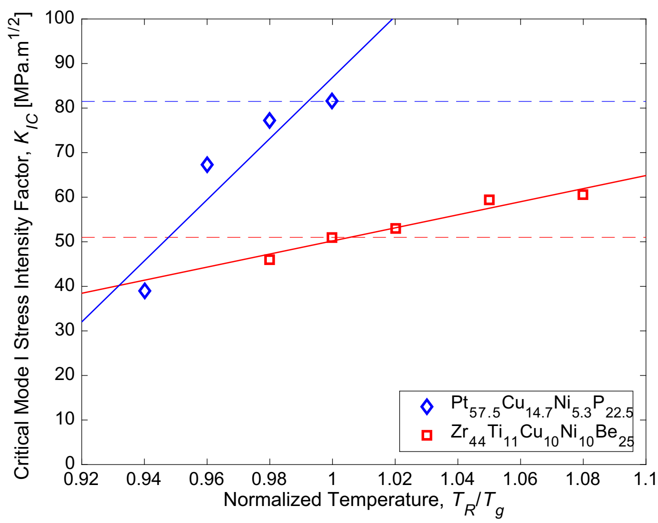

Fig. S2. Evaluated K_{IC} data for $Pt_{57.5}Ni_{5.3}Cu_{14.7}P_{22.5}$ and $Zr_{44}Ti_{11}Cu_{10}Ni_{10}Be_{25}$ using Eq. **S1** plotted against normalized temperature T_R/T_g. Solid lines are linear fits to the data. The upper dotted line designates the $K_{IC,g}$ value of 81.5 MPa·m$^{1/2}$ for $Pt_{57.5}Ni_{5.3}Cu_{14.7}P_{22.5}$ (33), whereas the lower dotted line designates the $K_{IC,g}$ value of 51 MPa·m$^{1/2}$ for $Zr_{44}Ti_{11}Cu_{10}Ni_{10}Be_{25}$ (11).

Table S1. Model parameters used in the present analysis to evaluate K_{IC} from the reported ε_f data using Eq. S1

Model parameters	$Pt_{57.5}Ni_{5.3}Cu_{14.7}P_{22.5}$	$Zr_{44}Ti_{11}Cu_{10}Ni_{10}Be_{25}$	Refs.
h, mm	0.3	0.3	(15)
ε_y	0.0153	0.020	(33, 34)
G_g, GPa	30.5	33.2	(21)
n	1.29	0.93	(21)
B, GPa	198.7	108.2	(33, 35)
$K_{IC,g}$, MPa·m$^{1/2}$	81.5	51	(33, 11)
Δu^*, µm	4.4	1.3	